Tailoring discrete quantum walk dynamics via extended initial conditions: Towards homogeneous probability distributions

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We study the evolution of initially extended distributions in the coined quantum walk on the line by analyzing the dispersion relation of the process and its associated wave equations. This allows us, in particular, to devise an initially extended condition leading to a uniform probability distribution whose width increases linearly with time, with increasing homogeneity.

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Introduction.– The discrete, or coined, quantum walk (QW) [1] is a process originally introduced as the quantum counterpart of the classical random walk (RW). In both cases there is a walker and a coin: at every time step the coin is tossed and the walker moves depending on the toss output. In the RW the walker moves to the right *or* to the left, while in the QW, as the walker and coin are quantum in nature, coherent superpositions right/left and head/tail happen. This feature endows the QW with outstanding properties, such as making the standard deviation of the position of an initially localized walker grow linearly with time t, unlike the RW in which this growth goes with $t^{1/2}$. This has strong consequences in algorithmics and is one of the reasons why QWs are receiving so much attention from the past decade. However the relevance of QW's is being recognized to go beyond this specific arena and, for example, some simple generalizations of the standard QW have shown unsuspected connections with phenomena such as Anderson localization [2] and quantum chaos [3, 4]. Moreover, theoretical and experimental studies evidence that the QW finds applications in outstanding systems, such as Bose–Einstein condensates [5], atoms in optical lattices [6, 7], trapped ions [8, 9], or optical devices [10–14], just to mention a few. This enhances the relevance of the QW as it can constitute a means for controlling the performance of those systems. Apart from the discrete QW we consider here, continuous versions exist as well [15], whose relationship with the coined QW has been discussed in [16].

Surprisingly enough even the simplest version of the discrete QW has not been studied in all its extension. Specifically we refer to the fact that in almost all studies up to date, the initial state of the walker is assumed to be sharply localized at the line origin, with few exceptions. In [16] it was shown that for wider initial distributions (an extended wavepacket), the evolution of the wavepacket is Gaussian-like, not showing the two characteristic outer peaks appearing in the probability distribution for more sharply localized initial conditions. In [6] also extended distributions, with top-hat profile, were considered in the context of the superfluid-Mott insulator transition in optical lattices, but no general conclusions were drawn on the influence of these extended initial conditions on the long time state. It is this issue that we address in this Letter, and the results we obtain open the way to new types of distributions that the QW can exhibit, e.g. virtually flat ones, with obvious impact in applications of this process.

The coined QW on the line.– In this QW the walker moves (at discrete time steps $t \in \mathbb{N}$) along a one-dimensional lattice of sites $x \in \mathbb{Z}$, with a direction that depends on the state of the coin (with eigenstates R and L). The state of the total system at (x,t) can be expressed in the form,

$$|\Psi_{x,t}\rangle = \mathrm{col}\left(R_{x,t}, L_{x,t}\right), \tag{1}$$

where $R_{x,t}$ and $L_{x,t}$ are wave functions on the lattice. As $|R_{x,t}|^2$ and $|L_{x,t}|^2$ have the meaning of probability of finding the walker at (x,t) and the coin in state R and L, respectively, the probability of finding the walker at (x,t) is

$$P_{x,t} = \langle\Psi_{x,t}\,|\Psi_{x,t}\rangle = |R_{x,t}|^2 + |L_{x,t}|^2, \tag{2}$$

and $\sum_x P_{x,t} = 1$. The QW is ruled by a unitary map and a standard form is [17]

$$R_{x,t+1} = R_{x+1,t}\cos\theta + L_{x+1,t}\sin\theta, \tag{3a}$$

$$L_{x,t+1} = R_{x-1,t}\sin\theta - L_{x-1,t}\cos\theta, \tag{3b}$$

where $\theta \in [0, \pi/2]$ is a parameter defining the bias of the coin toss ($\theta = \frac{\pi}{4}$ for an unbiased, or Hadamard, coin).

The dispersion relation and the group velocity.– Plane wave solutions to (3) exist in the form [18] $\exp\left[i\left(kx - \omega^{(s)}t\right)\right]\left|\Phi_k^{(s)}\right\rangle$, where $s = \pm$, $k \in [-\pi, +\pi]$, $\omega^{(+)} = \omega$, $\omega^{(-)} = \pi - \omega$,

$$\omega = -\arcsin\left(\cos\theta\sin k\right) \in \left[-\tfrac{\pi}{2}, \tfrac{\pi}{2}\right], \tag{4}$$

$$\left|\Phi_k^{(\pm)}\right\rangle = \mathcal{N}_\pm\,\mathrm{col}\left(\cos\theta\cos k \pm \cos\omega, e^{-ik}\sin\theta\right), \tag{5}$$

and $\mathcal{N}_\pm$ is a normalization factor (any $\mathcal{N}$ will have this meaning in the following). The dispersion relation (4) is represented in Fig. 1 together with the group velocity $v_{\mathrm{g}}^{(+)}(k) = d\omega/dk$ associated with $\left|\Phi_k^{(+)}\right\rangle$ [19]. The

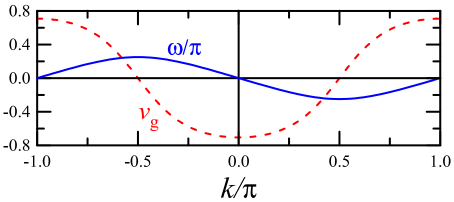

FIG. 1: (Colour online) Dispersion relation (full line) as given by Eq. (4), and corresponding group velocity (dashed line). $\theta=\pi/4$.

QW group velocity has been used for determining hitting times [20], and it will allow us to make simple but relevant predictions about the QW dynamics when the initial state is a wavepacket close to some of the eigensolutions above, say $\left|\Psi_{x,0}\right\rangle = f_x^{(s)} e^{ik_0x} \left|\Phi_{k_0}^{(s)}\right\rangle$ with $f_x^{(s)}$ a smooth envelope. In that case, as in any linear wave system, one must expect that, to the leading order, the group velocity govern its propagation. Hence if $k_0=\pm\pi/2$ a sufficiently extended wavepacket should stay at rest because $v_{\mathrm{g}}^{(s)}(\pm\pi/2)=0$, while if $k_0=0$ it should move with maximum velocity $v_{\mathrm{g}}^{(s)}(0)=-s\cos\theta$. If the initial condition projects onto both $\left|\Phi_{k_0=0}^{(\pm)}\right\rangle$ we must expect that the initial wavepacket splits into two, moving at opposite velocities given by $\mp\cos\theta$. Numerical simulations of the QW (with Gaussian initial conditions, see below) confirm these notable effects and tell us that the dispersion relation is a powerful tool for predicting QW dynamics [20]. As we demonstrate in the next sections the dispersion relation (4) controls not only the velocity of the wavepacket, but also the evolution of its shape as time runs, what will allow us making interesting predictions.

Broad initial distributions: Wave equations in the continuum limit.– The goal of this section is to find a wave equation for the wavepacket envelope with the help of discrete Fourier analysis. Given a function f_x on integers $x\in\mathbb{Z}$, one can define its discrete Fourier transform (DFT) as $\tilde{f}_k=\sum_x f_x e^{-ikx}$, which can be inverted as $f_x=(2\pi)^{-1}\int_{-\pi}^{+\pi}dk\tilde{f}_k e^{ikx}$. Applying this DFT to the map (3) it is straightforward to get an explicit solution to the QW given an arbitrary initial condition $\left|\Psi_{x,0}\right\rangle$. The result is $\left|\Psi_{x,t}\right\rangle=\sum_{s=\pm1}\left|\Psi_{x,t}^{(s)}\right\rangle$, where

$$\left|\Psi_{x,t}^{(s)}\right\rangle = \int_{-\pi}^{+\pi}\frac{dk}{2\pi}e^{i\left(kx-\omega^{(s)}t\right)}\left|\Phi_k^{(s)}\right\rangle\left\langle\Phi_k^{(s)}\right|\left.\tilde{\Psi}_{k,0}\right\rangle, \quad (6)$$

and $\left|\tilde{\Psi}_{k,0}\right\rangle=\sum_x e^{-ikx}\left|\Psi_{x,0}\right\rangle$.

As stated, we are interested in initial conditions of the form $\left|\Psi_{x,0}\right\rangle=\sum_{s=\pm1}f_x^{(s)}e^{ik_0x}\left|\Phi_{k_0}^{(s)}\right\rangle$, where the envelopes $f_x^{(s)}$ vary smoothly on x, and k_0 is a (carrier) wave number. Then $\left|\tilde{\Psi}_{k,0}\right\rangle=\sum_{s=\pm1}\tilde{f}_{k-k_0}^{(s)}\left|\Phi_{k_0}^{(s)}\right\rangle$, which is peaked around $k=k_0$ as $\tilde{f}_{k-k_0}^{(s)}$ is peaked around $k-k_0=0$ (low frequency envelope). In such cases Eq. (6) can be written as

$$\left|\Psi_{x,t}^{(s)}\right\rangle = e^{i\left(k_0x-\omega_0^{(s)}t\right)}F_s(x,t)\left|\Phi_{k_0}^{(s)}\right\rangle+\mathcal{O}(\Delta k), \quad (7)$$

$$F_s(x,t)=\int_{-\pi}^{+\pi}\frac{dK}{2\pi}\tilde{f}_K^{(s)}e^{i(Kx-s\Omega t)}, \quad (8)$$

where Δk is the width of $\tilde{f}_k^{(s)}$, $K=k-k_0$, $\Omega=\omega-\omega_0$, and we did not modify the limits of the integral because of the assumed smallness of Δk. We have introduced two wave functions, $F_\pm(x,t)$, in terms of which $P_{x,t}=\sum_{s=\pm1}\left|F_s(x,t)\right|^2+\mathcal{O}(\Delta k)$. We let $F_s(x,t)$ be defined on the reals, as there is nothing against that in Eq. (8), so that it is straightforward setting a wave equation from that equation,

$$i\partial_t F_s(x,t)=-is\omega_1\partial_x F_s-\tfrac{1}{2}s\omega_2\partial_x^2F_s+\cdots, \quad (9)$$

after Taylor expanding Ω around k_0, and where $\omega_n=\left(d^n\omega/dk^n\right)_{k=k0}$. This equation is to be solved under the initial condition $F_s(x,0)=f_x^{(s)}$ at integer x [22].

Eq. (9) is a main result of this Letter. It evidences the role played by the dispersion relation (4) as anticipated: For distributions whose DFT is centered around some k_0, the local variations of ω around k_0 determine the type of wave equation controlling the QW dynamics. The first term on the rhs gives the group velocity, already discussed, the second accounts for diffraction, and so on.

Application to Gaussian initial distributions.– Two cases of interest of Eq. (9) are analyzed next, corresponding to $k_0=0,\pi/2$ as suggested by the analysis of the dispersion relation. First, the case $k_0=0$ yields, to the leading order,

$$\partial_t F_s=(s\cos\theta)\,\partial_x F_s. \quad (10)$$

According to (10), if the (broad) initial condition projects onto both eigenspinors $\left|\Phi_0^{(\pm)}\right\rangle$, two wavepackets (whose height will depend on the projections $\left\langle\Phi_0^{(\pm)}\right.\left|\Psi_{x,0}\right\rangle$) will propagate without distortion at equal but opposite velocities given by $v_{\mathrm{g}}^{(s)}(0)=-s\cos\theta$ as commented above. We have checked this prediction in the original QW map (3) with initial states of the form $\left|\Psi_{x,0}\right\rangle=\mathcal{N}\exp\left[-\frac{1}{2}\left(x/\sigma_0\right)^2\right]\left|C\right\rangle$, which is a Gaussian of width σ_0. The state $\left|C\right\rangle$ of the coin (taken equal at any site) controls the projections $\left\langle\Phi_0^{(\pm)}\right.\left|\Psi_{x,0}\right\rangle$. The distortionless propagation at a velocity $v_{\mathrm{g}}^{(s)}(0)$ is observed in excellent agreement with the prediction even for moderate values of σ_0. Nevertheless, in all cases, a deformation of the wavepackets is visible after some running time, the longer the wider the initial distribution is. This deformation is controlled by the next, third order derivative term, in which case one has an equation similar to that derived in [10], where the role of the third order derivative was analyzed. This type of approximation was shown to be quite

good even for localized initial conditions, where the truncation of the dispersion relation is not so well justified as the initial condition projects over all k values.

The case $k_0 = \pi/2$ is more interesting for our purposes. It is described, to the leading order, by

$$i\partial_t F_s = -\frac{s}{2\tan\theta}\partial_x^2 F_s, \tag{11}$$

which is analogous to the Schrödinger equation as well as to the equation of paraxial optical diffraction, and the pulse propagation equation in linear optical fibers. The solution to (11) under Gaussian initial condition is $F_s(x,t) = \mathcal{N}\exp\left[-\frac{1}{2}(x-x_0)^2/(\sigma_0 q_s)^2\right]$, where σ_0 is the initial width and x_0 is center of the distribution (that remains constant as the group velocity is null in the present case), and the complex parameter $q_s(t) = \sqrt{1+ist/\sigma_0^2\tan\theta}$. The probability $P_s(x,t) = \mathcal{N}\exp\left[-(x-x_0)^2/(\sigma_0 w)^2\right]$ thus remains Gaussian with $w(t) = \sqrt{1+(t/\sigma_0^2\tan\theta)^2}$ the width of the distribution relative to its initial width σ_0, which grows linearly with time as soon as $t \gtrsim 5\sigma_0^2\tan\theta$ (note that these results are independent of s). Again, numerical simulations of (3), now with $|\Psi_{x,0}\rangle = \mathcal{N}\exp\left[-(x/\sigma_0)^2/2 + i\pi x/2\right]|C\rangle$ are in excellent agreement with the analytical predictions.

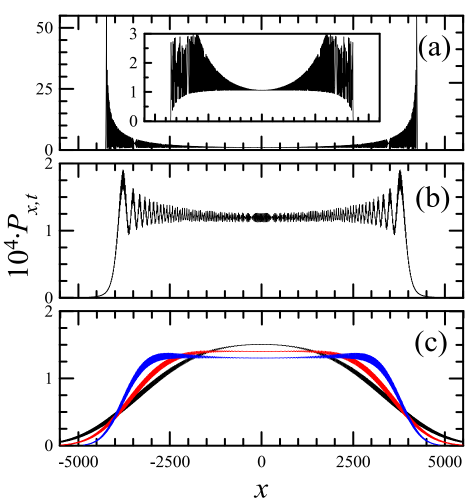

FIG. 2: Probability distributions for $\theta = \pi/4$ and different initial conditions. In (a) the initial condition is $|\Psi_{x,0}\rangle = \delta_{x,0}\left|\Phi^{(+)}_{\pi/2}\right\rangle$, fully localized at the origin, and the time run is $t = 6\times10^3$; the inset shows a magnification (odd sites have zero occupation probability). In (b) $|\Psi_{x,0}\rangle = \mathcal{N}\exp(i\pi x/2)\,\mathrm{sinc}(x/\sigma_0)\left|\Phi^{(+)}_{\pi/2}\right\rangle$ is used while in (c) additional Gaussians (of widths $\sigma_G = 1.1\sigma_0, 2\sigma_0$, and $3\sigma_0$, from top to bottom) multiply the initial condition; $\sigma_0 = 15$ and the time run is $t = 20\times10^3$.

Achieving homogeneous distributions.– In QW's a most desired result is that the probability distribution be as uniform as possible after a time. A hint towards that goal is given by light paraxial diffraction theory –that the QW follows for $k_0 = \pi/2$, Eq. (11): It is a textbook result that the far field corresponding to a light amplitude distribution $\mathrm{sinc}(x) = \sin(\pi x)/(\pi x)$ is remarkably homogeneous within a certain spatial region [23].

In order to gain insight into the problem we look at the solution to Eq. (11) under an initial condition $F(x,0) = \mathcal{N}\,\mathrm{sinc}(x/\sigma_0)$. This solution is obtainable by Fourier transformation of the spatial coordinate [24], $F_s(x,t) = \int_{-\infty}^{+\infty} dk\tilde{F}_s(k,0)\exp\left(ikx - isk^2t/2\tan\theta\right)$, with $\tilde{F}_s(k,0) = (2\pi)^{-1}\int_{-\infty}^{+\infty} dx F_s(x,0)\exp(-ikx)$. In our case $\tilde{F}_s(k,0) = (2\pi)^{-1}\sqrt{\sigma_0}\,\mathrm{rect}(\sigma_0 k/\pi)$, where $\mathrm{rect}(a) = 1$ if $|a| < 1$ and 0 otherwise. Hence $F_s(x,t) = (2\pi)^{-1}\sqrt{\sigma_0}\int_{-\pi/\sigma_0}^{+\pi/\sigma_0} dk\exp\left[it\phi_s(k,\xi)\right]$, with $\phi_s(k,\xi) = k\xi - sk^2/2\tan\theta$ and $\xi = x/t$.

As we are interested in the behavior of F_s at long times we can use the method of stationary phase [21] to evaluate the leading dependence of the integral on (x,t). It is straightforward to get $F_s(x,t) = w(t)^{-1/2}\exp\left[-i\left(s\pi/4 + x^2\tan\theta/2t\right)\right]$ with $w(t) = 2\pi(\sigma_0\tan\theta)^{-1}t$. Hence the asymptotic analysis predicts a uniform probability $P_s(x,t) = w(t)\,\mathrm{rect}\left[2x/w(t)\right]$, inside a segment of width $w(t)$. Thus we should expect, after a transient time (that can be estimated as $t \gtrsim 2\sigma_0^2\tan\theta$), a flat distribution whose width increases *linearly* with time (its standard deviation is $w(t)/\sqrt{12}$).

Inspired by this result we consider the actual QW initial condition $|\Psi_{x,0}\rangle = \mathcal{N}\exp(i\pi x/2)\,\mathrm{sinc}(x/\sigma_0)\left|\Phi^{(+)}_{\pi/2}\right\rangle$ with σ_0 the initial width. Figure 2(b) shows results of the simulation of (3), which are in qualitative agreement with the discussion above: A quite uniform distribution is attained. For comparison, the well known result corresponding to an initially localized distribution is shown in Fig. 2(a). Main differences are the improved degree of uniformity in (b), which is free from the large outer peaks in (a), and the fact that in (a) even/odd sites have null occupation probability at odd/even times unlike in (b). There is however a disgusting feature in (b), namely the high frequency ripples that appear at the plateau. Nevertheless the situation can be improved by multiplying the initial condition by a Gaussian of convenient width (this is a kind of smoothing processing, typical of optical diffraction [23]), as shown in Figure 2(c), which is another main result of this Letter: Almost uniform distributions (even reaching a top hat profile) can be obtained in the QW by making a judicious choice of the initial condition. We want to stress that these homogeneous distributions are so after a short transient, their homogeneity increasing with time.

The achievement of QW homogenous distributions is a most desired property. From the very beginning the relatively high homogeneity of the probability distribution of the QW corresponding to a localized initial condition has been considered as a positive quality of this process for information purposes. In [25] the presence of some de-

coherence in the process was considered to be beneficial because it leads to more homogeneous distributions *at a special time*. In this sense our finding may have relevance as we have seen that a judicious initial condition helps in achieving distributions with much larger and permanent homogeneity than the initially localized case, even including decoherence, as Fig. 2(c) clearly demonstrates.

Conclusions and discussion.– In this work we have studied the influence of the initial condition on the discrete QW on the line guided by the QW dispersion relation and by its associated wave equations. Specifically we have considered the evolution of initially extended probability distributions. We have shown that sufficiently wide Gaussian initial distributions propagate without distortion and small width increase at velocities that can be tuned, including null velocity, with a proper choice of the phases along the initial distribution as given by the phase factor $\exp(ik_0x)$. We have devised as well an initial condition that leads, after a transient, to a homogeneous distribution whose width increases with time remaining highly homogeneous at any later time. This result, Fig. 2(c), is a main result of this paper.

We further mention that any behavior of light diffraction (or linear pulse propagation) can be transferred to the QW in the case of the resting probability distributions ($k_0 = \pi/2$), as its continuous limit, Eq. (11), is nothing but the paraxial diffraction equation. For instance, a light pattern replicates at specific planes when it is periodic, the so called Talbot effect [23]. In our case, if $F_s(x+\lambda,0) = F_s(x,0)$, where λ is the spatial period, then $|F_s(x,nT)|^2 = |F_s(x,0)|^2$, where $T = (2\pi)^{-1}\lambda^2\tan\theta$ is the Talbot period and n is integer. Other optical effects, such as those of lenses, can also be mimicked by introducing quadratic phase factors [23] in the initial condition. It is just the choice of that condition that can make any paraxial, linear optical phenomenon be reproduced with the QW, what can be useful for special implementations of this rich process.

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[22] According to (8) $F_s(x,0) = (2\pi)^{-1}\int_{-\pi}^{+\pi} dK \tilde{f}_K^{(s)} \exp(iKx) = \sum_y f_y^{(s)} \operatorname{sinc}(x-y)$, where $\operatorname{sinc}(x) = \sin(\pi x)/(\pi x)$, and at integer x $\operatorname{sinc}(x-y) = \delta_{x,y}$. In general the relation between $f_x^{(s)}$ and $F_s(x,0)$ is not invertible, what means that not all the choices for the latter correspond to a true $f_x^{(s)}$. However, any choice of $F_s(x,0)$ varying smoothly on the unit spatial scale corresponds to a true $f_x^{(s)} = F_s(x,0)$ at integer x.

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